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Science & Emerging Technology of 2D Atomic Layered Materials and Devices

Angel Rubio
UNIVERSIDAD DEL PAIS VASCO - EUSKAL HERRIKO UNIBERTSITTEA

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Final Report

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14. ABSTRACT <p>The project resulted in 16 published papers in world-class journals and was instrumental, directly or indirectly, in the award of nine prestigious Marie Sklodowska-Curie grants to pursue follow-on research.</p> <p>The papers that describe all the work are accessible in the attached document and are listed here:</p> <ul style="list-style-type: none"> - Creating stable Floquet-Weyl semimetals by laser-driving of 3D Dirac materials. - h-AlN-Mg(OH)₂ vdW Bilayer Heterostructure: Tuning the excitonic characteristics - Emergent elemental two-dimensional materials beyond grapheme. - Ab Initio Modeling of Plasmons in Metal-Semiconductor Bilayer Transition Metal Dichalcogenide Heterostructure - Atoms and Molecules in Cavities: From Weak to Strong Coupling in QED Chemistry. - Confined linear carbon chains as a route to bulk carbyne - On the exciton coupling between two chlorophyll pigments in the absence of a protein environment: Intrinsic effects revealed from theory and experiment. - Square selenene and tellurene: novel group VI elemental 2D semi-Dirac materials and topological insulators. - Quantum Plasmonics: From jellium models to ab-initio calculations. - Negative plasmon dispersion in 2H-NbS₂ beyond charge-density-wave interpretation - Stable monolayer honeycomb-like structures of RuX₂ (X = S, Se). - Disentangling Vacancy Oxidation on Metallicity-Sorted Carbon Nanotubes. - Theoretical Insight into the Internal Quantum Efficiencies of Polymer/C60 and Polymer/SWNT Photovoltaic Devices. - Dynamics of observables and exactly solvable quantum problems: Using time-dependent density functional theory to control quantum systems. 					
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Dr. Misoon Mah
Asian Office of Aerospace Research and Development
45002, APO AP 96337-5002
7-23-17 Roppongi, Minato-ku
Tokyo, Japan 106-0032

March 8, 2017

Dear Dr. Mah,

Please find the attached forms SF-425-FFR and dd082, which constitutes the final reporting documents for AOARD project 144088, "2D Materials and Devices Beyond Graphene Science & Emerging Technology of 2D Atomic Layered Materials and Devices". These documents cover the grant period from February 19, 2016-February 18, 2017

We are proud to note that this AOARD funding contributed to the production of the following publications:

[Creating stable Floquet-Weyl semimetals by laser-driving of 3D Dirac materials](#)

Hannes Hübener, Michael A. Sentef, Umberto De Giovannini, Alexander F. Kemper, Angel Rubio
Nature Communications **7**, 13940 (2017)

[h-AIN-Mg\(OH\)2 vdW Bilayer Heterostructure: Tuning the excitonic characteristics](#)

C. Bacaksiz, A. Dominguez, A. Rubio, R. T. Senger, H. Sahin
Physical Review B **(accepted)**, (2017)

[Emergent elemental two-dimensional materials beyond graphene](#)

Yuanbo Zhang, Angel Rubio, Guy Le Lay
Journal Of Physics D-Applied Physics **50**, 053004 (11pp) (2017)

[Ab Initio Modeling of Plasmons in Metal-Semiconductor Bilayer Transition Metal Dichalcogenide Heterostructure](#)

Huseyin Sener Sen, Lede Xian, Felipe Homrich da Jornada, Steven Louie, Angel Rubio
Israel Journal of Chemistry **(2017)**

[Atoms and Molecules in Cavities: From Weak to Strong Coupling in QED Chemistry](#)

Johannes Flick, Michael Ruggenthaler, Heiko Appel, Angel Rubio
(2017)

[Confined linear carbon chains as a route to bulk carbyne](#)

L. Shi, P. Rohringer, K. Suenaga, Y. Niimi, J. Kotakoski, J.C. Meyer, H. Peterlik, M. Wanko, S. Cahangirov, A. Rubio, Z.J. Lapin, L. Novotny, P. Ayala, T. Pichler
Nature Materials **15**, 634 - 639 (2016)

[On the exciton coupling between two chlorophyll pigments in the absence of a protein environment: Intrinsic effects revealed from theory and experiment](#)

Dr. Bruce F. Milne, Christina Kjær, Jørgen Houmøller, Dr. Mark H. Stockett, Dr. Yoni Toker, Prof. Angel Rubio, Prof. Steen Brøndsted Nielsen
Angewandte Chemie International Edition **128**, 6356 - 6359 (2016)

[Square selenene and tellurene: novel group VI elemental 2D semi-Dirac materials and topological insulators](#)

Lede Xian, Alejandro Pérez Paz, Elisabeth Bianco, Pulickel M. Ajayan, Angel Rubio
Physical Review Letters **(Submitted)**, (2016)

[Quantum Plasmonics: From jellium models to ab-initio calculations](#)

Alejandro Varas, Pablo García-González, Johannes Feist, F. J. García-Vidal, Angel Rubio
Nanophotonics **5**, 409 - 426 (2016)



Negative plasmon dispersion in 2H-NbS₂ beyond charge-density-wave interpretation

Pierluigi Cudazzo, Eric Müller, Carsten Habenicht, Matteo Gatti, Helmuth Berger, Martin Knupfer, Angel Rubio, Simo Huotari
New Journal Of Physics **18**, 103050 (2016)

Stable monolayer honeycomb-like structures of RuX₂ (X = S, Se)

Ersan, Fatih; Cahangirov, Seymur; Gokoglu, Gokhan; et al.
Physical Review B **94**, 155415 (2016)

Disentangling Vacancy Oxidation on Metallicity-Sorted Carbon Nanotubes

Duncan J. Mowbray, Alejandro Pérez Paz, Georgina Ruiz-Soria, Markus Sauer, Paolo Lacovig, Matteo Dalmiglio, Silvano Lizzit, Kazuhiro Yanagi, Andrea Goldoni, Thomas Pichler, Paola Ayala, Angel Rubio
Journal Of Physical Chemistry C **120** (32), pp 18316–18322 (2016)

Theoretical Insight into the Internal Quantum Efficiencies of Polymer/C₆₀ and Polymer/SWNT Photovoltaic Devices

Livia Noemi Glanzmann, Duncan John Mowbray
Journal Of Physical Chemistry C **120**, 6336 - 6343 (2016)

Dynamics of observables and exactly solvable quantum problems: Using time-dependent density functional theory to control quantum systems

Mehdi Farzanehpour, I. V. Tokatly
Physical Review A **93**, 052515 (2016)

Tailored pump-probe transient spectroscopy with time-dependent density-functional theory: controlling absorption spectra

J. Walkenhorst, U. De Giovannini, A. Castro, A. Rubio
European Physical Journal B **89**, 128 (2016)

Anisotropic electronic, mechanical and optical properties of monolayer WTe₂

E. Torun, H. Sahin, S. Cahangirov, A. Rubio, F. M. Peeters
Journal Of Applied Physics **119**, 074307 (2016)

In addition, the work that was performed under this grant was instrumental in assisting us, directly or indirectly, in obtaining the following nine prestigious Marie Skłodowska-Curie grants:

Marie Curie Intra-European Fellowships (IEF) (FP7-PEOPLE-2013-IEF, Project 622934) "Optical charge transfer processes in early stages of photosynthesis from first-principle computational techniques" (OptChaTra) Dr. Hannes Huebener (2014-2016). (Total: 166,336€)

Marie Curie Intra-European Fellowships (IEF) (FP7-PEOPLE-2013-IEF, Project 628876 "Photophysics of Fluorescent Proteins" (PhotoProtein). Dr. Seymur Cahangirov (2014-2016)- (Total: 173,370€)

Marie Curie Individual Fellowship (IF) (H2020-MSCA-IF-2014, Project 660231 "Electrical Spin Manipulation in Atoms and Molecules" (SpinMan). Dr. Andrea Droghetti (2016-2018). (Total: 158,122€)

Marie Curie Individual Fellowship (IF) (H2020-MSCA-IF-2014, Project SEP-210195067 "Quantum Effects in Multicolor Ultrafast Laser Processing: Broadening Boundaries of Classical Descriptions" (QuantumLaP). Dr. Derrien Thibault (2015-2017). (Total: 142,721€)

Marie Curie Individual Fellowship (IF) (H2020-MSCA-IF-2015, Project 702406 "Correlated Electron-Nuclear Dynamics: A novel mixed quantum-semiclassical approach (CoEND)". Dr. Ali Abedi (2016-2018). (Total: 170,121.60 €)

Marie Curie Individual Fellowship (IF) (H2020-MSCA-IF-2015, Project 704218 "Strong Field Dynamics of Atoms and Molecules: History-dependent Functionals and Exact Kohn-Sham Potentials of the Time-dependent (multi-component) Density Functional Theory (AMO-dance)", Dr. Elham Khosravi (2016-2018). (Total: 170,121.60 €)

Marie Curie Individual Fellowship (IF) (H2020-MSCA-IF-2015, Project 706890 "Thermodynamics of Quantum Transport (QFluctTrans)". Dr. Cesar A. Rodriguez-Rosario (2016-2018). (Total: 170,121.60 €)



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Marie Curie Individual Fellowship (IF) (H2020-MSCA-IF-2015, Project 703195 "Spin-Orbit Coupling at Interfaces from Spintronics to new Superconducting effects (SOCISS)". Dr. Juan Borge de Prada (2016-2018). (Total: 158,121.60 €)

Marie Curie Individual Fellowship (IF) (H2020-MSCA-IF-2016, Project 753874 "Excitonic quasiparticles in Titania (exciTitania)". Dr. Adriel Dominguez (2017-2019). (Total: 158,121 €)

We greatly appreciate the support of the AOARD. Please contact grants manager Kate Chabarek (kathryina.chabarek@ehu.eus) if you have any questions or concerns about the attached reports.

Many thanks.

Regards,

Angel Rubio
Distinguished Professor of Physics